Listing of the Claims:

1. (Previously Presented) A computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function;

(d) deconvoluting said M compounds into their associated building blocks;

(e) generating said focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting at least one K compound; and

(h) synthesizing said at least one K compound.

2. (Previously Presented) The method of claim 1, wherein said focused library of at least one compound includes a plurality of compounds, further comprising:

(i) selecting at least one K compound from said focused library of compounds, and outputting a list of said at least one K compound.

3. (Canceled)

4. (Canceled)

5. (Canceled)

6. (Canceled)

7. (Previously Presented) The method of claim 1, wherein the at least one fitness function in step (c) is selected from similarity, diversity, and presence or absence at least one characteristic.

8. (Previously Presented) The method of claim 7, wherein said focused library of at least one compound includes a plurality of compounds, wherein step (g) further comprises: selecting at least one K compound from said focused library of compounds based on said fitness function and outputting a list of said at least one K compound.

9. Cancelled

10. (Previously Presented) The method of claim 8, wherein step (c) comprises:

(i) selecting an initial sub-set of M compounds from said set of N enumerated compounds;

(ii) evaluating said initial sub-set of M compounds based on said fitness function; and

(iii) refining said initial sub-set of M compounds based on said fitness function, thereby selecting said M compounds.

11. (Previously Presented) The method of claim 10, wherein step (g) comprises:

(i) selecting an initial sub-set of at least one K compound from said focused library of compounds;

(ii) evaluating said initial sub-set of at least one K compounds based on said fitness function; and

(iii) refining said initial sub-set of at least one K compound based on the fitness function, thereby selecting said at least one K compound.

12. (Previously Presented) The method of claim 11, wherein said fitness function is related to diversity of a collection of compounds, and wherein step (c)(ii) comprises evaluating a diversity of said initial sub-set of M compounds, and wherein step (c)(iii) comprises refining said initial sub-set of M compounds to increase said diversity of said M compounds

13. (Previously Presented) A computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function selected from similarity, diversity, and presence or absence at least one characteristic wherein selection comprises:

(i) selecting an initial sub-set of M compounds from said set of N enumerated compounds;

(ii) evaluating said initial sub-set of M compounds based on said fitness function which comprises evaluating a diversity of said initial sub-set of M compounds; and

(iii) refining said initial sub-set of M compounds based on said fitness function to increase said diversity of said M compounds, thereby selecting said M compounds;

(d) deconvoluting said M compounds into their associated building blocks;

(e) generating said focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting at least one K compound from said focused library of compounds based on said fitness function by:

(i) selecting an initial sub-set of at least one K compound from said focused library of compounds;

(ii) evaluating said initial sub-set of at least one K compounds based on said fitness function thereby evaluating the diversity of said initial sub-set of K compounds ;

(iii) refining said initial sub-set of at least one K compound based on the fitness function to increase the diversity of said K compounds, thereby selecting said at least one K compound; and

(iv) outputting a list of said at least one K compound; and

(h) synthesizing said at least one K compound.

14. (Previously Presented) The method of claim 8, wherein step (c) comprises:

(i) characterizing said N enumerated compounds;

(ii) evaluating said characterized N enumerated compounds based on said fitness function;

(iii) ranking said characterized N enumerated compounds based on said evaluation; and

(iv) selecting said M compounds based on said ranking.

15. (Previously Presented) The method of claim 14, wherein said focused library of at least one compound comprises a plurality of compounds, wherein step (g) comprises:

(i) characterizing said compound of said focused library of compounds;

(ii) evaluating said characterized compound of said focused library of compounds based on said fitness function;

(iii) ranking said characterized compounds of said focused library of compounds based on said evaluation; and

(iv) selecting said K compounds based on said ranking.

16. (Previously Presented) The method of claim 15, wherein step (c)(i) comprises characterizing said N enumerated compounds using a set of molecular descriptors.

17. (Previously Presented) The method of claim 16, wherein step (g)(i) comprises characterizing compounds of said enumerated focused library of compounds using said set of molecular descriptors.

18. (Previously Presented) The method of claim 15, wherein said fitness function is related to a similarity to one or more query structures, and wherein step (c)(ii) comprises evaluating similarity between said N enumerated compounds and said one or more query structures.

19. (Previously Presented) The method of claim 18, wherein at least one of the following similarity measures is used in step (c)(ii) for evaluating similarity between each compounds and said one or more query structures:

(1) similarity in number of atoms, bonds and rings of the same types;

(2) similarity in shape and surface characteristics;

(3) similarity in electron density distribution;

(4) similarity based on common substructure;

(5) similarity based on the presence and orientation of pharmacophoric groups;

(6) similarity in binding affinity; and

(7) similarity in degree of conformational overlap with a know receptor binder.

20. (Previously Presented) A computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function selected from similarity, diversity, and presence or absence at least one characteristic whereby selection comprises:

(i) characterizing said N enumerated compounds;

(ii) evaluating said characterized N enumerated compounds based on said fitness function which is related to a similarity between said N enumerated compounds and said one or more query structures;

(iii) ranking said characterized N enumerated compounds based on said evaluation; and

(iv) selecting said M compounds based on said ranking.

(d) deconvoluting said M compounds into their associated building blocks;

(e) generating said focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting at least one K compound from said focused library of compounds based on said fitness function by :

(i) characterizing said compound of said focused library of compounds;

(ii) evaluating said characterized compound of said focused library of compounds based on said fitness function thereby evaluating similarity between compounds of said enumerated focused library of compounds and said one or more query structures wherein the same similarity measure is used for evaluating similarity in step (c)(ii);

(iii) ranking said characterized compounds of said focused library of compounds based on said evaluation;

(iv) selecting said K compounds based on said ranking; and

(v) outputting a list of said at least one K compound; and

(h) synthesizing said at least one K compound.

21. (Previously Presented) The method of claim 14, wherein said fitness function is related to at least one desired characteristic, and wherein step (c)(ii) comprises evaluating N enumerated compounds to determine an extent to which the N enumerated compounds possess the at least one desired characteristic.

22. (Previously Presented) The method of claim 21, wherein the at least one desired characteristic comprises at least one of the following:

(1) a desired physical property;

(2) a desired chemical property;

(3) a desired functional property; and

(4) a desired bioactive property.

23. (Previously Presented) A computer based system for analyzing a non-enumerated virtual library, comprising:

means for randomly selecting a set of N reagent combinations from the virtual library, wherein said selected N reagent combinations represent a set of N compounds;

means for enumerating said set of N compounds;

means for selecting M compounds of said set of N enumerated compounds based on a fitness function;

means for deconvoluting said M compounds into their associated building blocks;

means for generating a said focused library of compounds based on said building blocks;

means for enumerating a plurality of said compounds of said focused library of compounds; and

means for selecting at least one K compound of said enumerated compounds of said focused library based on the fitness function,

wherein at least one selected K compound is synthesized.

24. (Previously Presented) A computer program product comprising a computer useable medium having computer program logic recorded thereon for enabling a processor to analyze a non-enumerated virtual library, the computer program logic comprising:

a first function that enables the processor to randomly select a set of N reagent combinations from the virtual library, wherein said selected N reagent combinations represent a set of N compounds;

a second function that enables the processor to enumerate said set of N compounds;

a first function that enables the processor to select M compounds of said set of N enumerated compounds based on a fitness function;

a third function that enables the processor to deconvolute said M compounds into their associated building blocks;

a fourth function that enables the processor to generate said focused library based on said building blocks;

a fifth function that enables the processor to enumerate a plurality of said compounds of said focused library; and

a sixth function that enables the processor to select at least one K compound of said enumerated compounds of said focused library based on the fitness function,

wherein at least one selected K compound is synthesized.

25. (Previously Presented) A computer implemented method of analyzing an enumerated virtual library, comprising:

(a) randomly selecting a set of N enumerated compounds from the enumerated virtual library;

(b) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function:

(c) deconvoluting said M compounds into associated building blocks;

(d) extracting said enumerated focused library based on said building blocks; said enumerated focused library including S enumerated compounds;

(e) selecting at least one K compound from said S enumerated compounds, wherein $K < S$; and

(f) synthesizing said at least one selected K compound.

26. (Previously Presented) The method of claim 25, wherein step (e) further comprises outputting a list of said at least one K compound.

27. (Canceled)

28. (Canceled)

29. (Canceled)

30. (Canceled)

31. (Previously Presented) The method of claim 25, wherein the at least one fitness function in step (b) is selected from similarity, diversity, and presence or absence at least one characteristic.

32. (Previously Presented) The method of claim 31, wherein step (e) further comprises selecting at least one K compound from said S enumerated compounds based on said fitness function.

33. (Canceled)

34. (Previously Presented) The method of claim 32, wherein step (b) comprises:

(i) selecting an initial sub-set of M compounds from said set of N enumerated compounds;

(ii) evaluating said first sub-set of M enumerated compounds based on said fitness function; and

(iii) refining said initial sub-set of M enumerated compounds based on said fitness function, thereby selecting said M compounds.

35. (Previously Presented) The method of claim 34, wherein step (e) comprises:

(i) selecting an initial sub-set of at least one K compound from said S enumerated compounds;

(ii) evaluating said sub-set of at least one K compound based on said fitness function; and

(iii) refining said sub-set of at least one K compound based on said fitness function, thereby selecting said at least one K compound.

36. (Previously Presented) The method of claim 35, wherein said fitness function is related to a diversity of a collection of compounds, and wherein step (b)(ii) comprises evaluating a diversity of said sub-set of M enumerated compounds, and wherein step (b)(iii) comprises refining said sub-set of M enumerated compounds to increase the diversity of said sub set of M enumerated compounds.

37. (Previously Presented) The method of claim 36, wherein said initial sub-set of at least one K compound comprises a plurality of K compounds, wherein step (e)(ii) comprises evaluating the diversity of said initial sub-set of K compounds, and wherein step (e)(iii) comprises refining said initial sub-set of K compounds to increase the diversity of said K compounds.

38. (Previously Presented) The method of claim 32, wherein step (b) comprises:

(i) characterizing said set of N enumerated compounds;

(ii) evaluating said characterized set of N enumerated compounds based on said fitness function;

(iii) ranking said characterized set of N enumerated compounds; and

(iv) selecting said M compound of said set of N enumerated compounds based on said ranking.

39. (Previously Presented) The method of claim 38, wherein step (e) comprises:

(i) characterizing said S enumerated compounds;

(ii) evaluating said characterized S enumerated compounds based on said fitness function;

(iii) ranking said characterized S enumerated compounds; and

(iv) selecting said at least one K compound of said S enumerated compounds based on said ranking.

40. (Previously Presented) The method of claim 39, wherein step (b)(i) comprises characterizing said set of N enumerated compounds using a set of molecular descriptors.

41. (Previously Presented) The method of claim 40, wherein step (b)(i) comprises characterizing said S enumerated compounds using said set of molecular descriptors,

42. (Previously Presented) The method of claim 38, wherein said fitness function is related to a similarity to one or more query structures, and wherein step (b)(ii) comprises evaluating a similarity between compounds of said set of N enumerated compounds and the one or more query structures.

43. (Previously Presented) The method of claim 42, wherein at least one of the following similarity measures is used in step (b)(ii) for evaluating similarity between said set of N enumerated compounds and the one or more query structures:

(1) similarity in number of atoms, bonds and rings of the same types;

(2) similarity in shape and surface characteristics;

(3) similarity in electron density distribution;

(4) similarity based on common substructure;

(5) similarity based on the presence and orientation of pharmacophoric groups;

(6) similarity in binding affinity; and

(7) similarity in degree of conformational overlap with a know receptor binder.

44. (Previously Presented) The method of claim 42, wherein step (e)(ii) comprises evaluating similarity between said S enumerated compounds and the one or more query structures, and wherein the same similarity measure is used for evaluating similarity in step (b)(ii) and step (e)(ii).

45. (Previously Presented) The method of claim 38, wherein said fitness function is related to at least one desired characteristic, and wherein step (b)(ii) comprises evaluating said set of N enumerated compounds to determine an extent that said N enumerated compounds possesses the at least one desired characteristic.

46. (Previously Presented) The method of claim 45, wherein said at least one desired characteristic comprises at least one of the following:

(1) a desired physical property;

(2) a desired chemical property;

(3) a desired functional property; and

(4) a desired bioactive property.

47. (Previously Presented) A computer based system for analyzing an enumerated virtual library, comprising:

means for randomly selecting a set of N enumerated from the enumerated virtual library;

means for selecting M compounds of said set of N enumerated compounds based on the fitness function;

means for deconvoluting said M compounds into their associated building blocks;

means for extracting an enumerated focused library, based on said associated building blocks from the enumerated virtual library, wherein said enumerated focused library includes S enumerated compounds; and

means for selecting at least one K compound of said S enumerated compounds based on the fitness function,

wherein at least one selected K compound is synthesized.

48. (Previously Presented) A computer program product comprising a computer useable medium having computer program logic recorded thereon for enabling a processor to analyze an enumerated virtual library, the computer program logic comprising:

a first function that enables the processor to randomly select a set of N enumerated compounds from the enumerated virtual library;

a second function that enables the processor to select M compounds of said set of N enumerated compounds based on the fitness function;

a third function that enables the processor to deconvolute said M compounds into associated building blocks;

means for extracting an enumerated focused library, based on said associated building blocks from the enumerated virtual library, wherein said enumerated focused library includes S enumerated compounds; and

a fourth function that enables the processor to select at least one K compound of said S enumerated compounds based on the fitness function; and

a fifth function that enables the processor to select at least one K compound from said S enumerated compounds, wherein $K < S$, wherein at least one selected K compound is synthesized.